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=> b reg
FILE 'REGISTRY' ENTERED AT 14:48:58 ON 17 AUG 2009
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STRUCTURE FILE UPDATES:   16 AUG 2009  HIGHEST RN 1174375-84-8
DICTIONARY FILE UPDATES:  16 AUG 2009  HIGHEST RN 1174375-84-8

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experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

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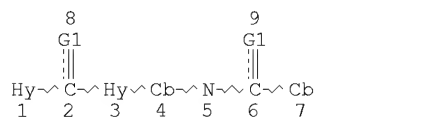


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GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
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STEREO ATTRIBUTES: NONE
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100.0% PROCESSED     159 ITERATIONS                          14 ANSWERS
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FILE 'ZCAPLUS' ENTERED AT 14:49:04 ON 17 AUG 2009
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FILE COVERS 1907 - 17 Aug 2009  VOL 151 ISS 8
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FILE LAST UPDATED: 16 Aug 2009 (20090816/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2009

ZCAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2009.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate substance identification.

The ALL, BIB, MAX, and STD display formats in the CA/CAplus family of databases have been updated to include new citing references information. This enhancement may impact record import into database management software. For additional information, refer to NEWS 9.

=> d bib abs hitstr l17 tot

L17 ANSWER 1 OF 2 ZCAPLUS COPYRIGHT 2009 ACS on STN
AN 2005:823712 ZCAPLUS
DN 143:229891
TI Diazabicyclic aryl derivatives as nicotinic acetylcholine receptor ligands, their preparation and pharmaceutical compositions
IN Peters, Dan; Olsen, Gunnar M.; Nielsen, Elsebet Ostergaard; Jorgensen, Tino Dyhring; Anring, Philip K.; Timmermann, Daniel B.
PA Neurosearch A/S, Den.
SO PCT Int. Appl., 49 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

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PI WO--2005075482	A1	20050818	2005WO-EP0050405	20050201
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2005WO-EP0050405	W	20050201		

OS CASREACT 143:229891; MARPAT 143:229891
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention relates to a group of diazabicyclic aryl derivs. I, including its enantiomers, N-oxides, prodrugs, and pharmaceutically acceptable salts, which are cholinergic ligands at the nicotinic acetylcholine receptors. In compds. I, n is 1-3; X and Y are independently selected from (un)substituted aromatic monocyclic/polycyclic carbocycles/heterocycles; Z is an (un)substituted monocyclic heterocycle, amino, (thio)carbonylamino, imidamido, ureido, thioureido, or guanidino; and L is a bond, CH2, CH2CH2, CH=CH, C.tplbond.C, O, S, SCH2, etc. The invention also relates to the preparation of I, pharmaceutical comps. containing I or a pharmaceutically acceptable salt of I, together with at least one pharmaceutically acceptable carrier or diluent, as well as to the use of the comps. for the treatment of diseases and disorders associated with nicotinic acetylcholine receptors. 3-Quinuclidinone hydrochloride was condensed with hydroxylamine and ring expansion followed by reduction with LiAlH4 resulted in the formation of 1,4-diazabicyclo[3.2.2]nonane (II). II was acylated with 5-(4-nitrophenyl)-2-furoyl chloride (preparation in situ from the corresponding acid is given) to give III. Palladium-catalyzed hydrogenation of III followed by addition to Et isocyanate gave diazabicyclic derivative IV. Compound IV expressed IC50 value of 0.56 nM in a study on the

L17 ANSWER 1 OF 2 ZCAPLUS COPYRIGHT 2009 ACS on STN (Continued)
inhibition of [3H]-α-bungarotoxin in rat brain, representing the α7-subtype of nicotinic receptors.
IT **753499-87-5P**, N-[4-[5-[(1,4-Diazabicyclo[3.2.2]non-4-yl)carbonyl]furan-2-yl]phenyl]benzamide **862851-87-4P**, 4-Amino-N-[4-[5-[(1,4-diazabicyclo[3.2.2]non-4-yl)carbonyl]furan-2-yl]phenyl]benzamide **862851-89-6P**, 3-Amino-N-[4-[5-[(1,4-diazabicyclo[3.2.2]non-4-yl)carbonyl]furan-2-yl]phenyl]benzamide **862852-29-7P**, N-[3-[5-[(1,4-Diazabicyclo[3.2.2]non-4-yl)carbonyl]furan-2-yl]phenyl]benzamide **862852-30-0P** **862852-33-3P**, N-[4-[5-[(1,4-Diazabicyclo[3.2.2]non-4-yl)carbonyl]furan-2-yl]phenyl]-2-nitrobenzamide hydrochloride **862852-43-5P**, N-[4-[5-[(1,4-Diazabicyclo[3.2.2]non-4-yl)carbonyl]furan-2-yl]phenyl]-2-nitrobenzamide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of diazabicyclic aryl derivs. as nicotinic acetylcholine receptor ligands)
RN 753499-87-5 ZCAPLUS
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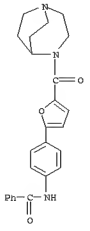

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L17 ANSWER 1 OF 2 ZCAPLUS COPYRIGHT 2009 ACS on STN (Continued)
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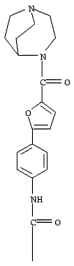

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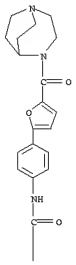
PAGE 1-A



L17 ANSWER 1 OF 2 ZCAPLUS COPYRIGHT 2009 ACS on STN (Continued)
PAGE 2-A

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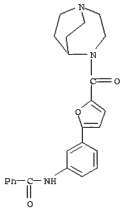

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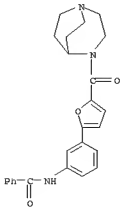
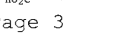


CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



L17 ANSWER 1 OF 2 ZCAPLUS COPYRIGHT 2009 ACS on STN (Continued)

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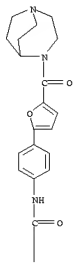
PAGE 1-A



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● HCl

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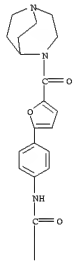
L17 ANSWER 1 OF 2 ZCAPLUS COPYRIGHT 2009 ACS on STN (Continued)

PAGE 1-A



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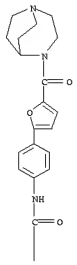
PAGE 1-A



L17 ANSWER 1 OF 2 ZCAPLUS COPYRIGHT 2009 ACS on STN (Continued)

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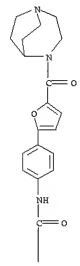

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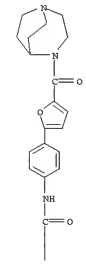
IT **862851-88-5P**, N-[4-[5-[(1,4-Diazabicyclo[3.2.2]non-4-yl)carbonyl]furan-2-yl]phenyl]-4-nitrobenzamide **862851-90-9P**, N-[4-[5-[(1,4-Diazabicyclo[3.2.2]non-4-yl)carbonyl]furan-2-yl]phenyl]-3-nitrobenzamide **862852-35-5P**, N-[4-[5-[(1,4-Diazabicyclo[3.2.2]non-4-yl)carbonyl]furan-2-yl]phenyl]-4-nitrobenzamide hydrochloride **862852-37-7P**, N-[4-[5-[(1,4-Diazabicyclo[3.2.2]non-4-yl)carbonyl]furan-2-yl]phenyl]-3-nitrobenzamide hydrochloride
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of diazabicyclic aryl derivs. as nicotinic acetylcholine receptor ligands)
RN 862851-88-5 ZCAPLUS
CN Benzamide, N-[4-[5-(1,4-diazabicyclo[3.2.2]non-4-ylcarbonyl)-2-furanyl]phenyl]-4-nitro- (CA INDEX NAME)

L17 ANSWER 1 OF 2 ZCAPLUS COPYRIGHT 2009 ACS on STN (Continued)

PAGE 2-A

RN 862852-35-5 ZCAPLUS
CN Benzamide, N-[4-[5-(1,4-diazabicyclo[3.2.2]non-4-ylcarbonyl)-2-furanyl]phenyl]-4-nitro-, hydrochloride (1:1) (CA INDEX NAME)

PAGE 1-A



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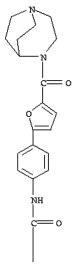
● HCl

RN 862852-37-7 ZCAPLUS
CN Benzamide, N-[4-[5-(1,4-diazabicyclo[3.2.2]non-4-ylcarbonyl)-2-furanyl]phenyl]-3-nitro-, hydrochloride (1:1) (CA INDEX NAME)

L17 ANSWER 1 OF 2 ZCAPLUS COPYRIGHT 2009 ACS on STN (Continued)

PAGE 1-A



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● HCl

OSC.G 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)
RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 2 OF 2 ZCAPLUS COPYRIGHT 2009 ACS on STN (Continued)
Et formate gave II in 53% yield. II showed inhibition of 3H-α-Bungarotoxine binding with IC50 value of 0.017μM. Thus, I and their pharmaceutical compns. are useful as cholinergic ligands at the nicotinic acetylcholine receptors for the treatment of the central nervous system (CNS), the peripheral nervous system (PNS), diseases or disorders related to smooth muscle contraction, endocrine diseases or disorders, diseases or disorders related to neuro-degeneration, diseases or disorders related to inflammation, pain, and withdrawal symptoms caused by the termination of abuse of chem. substances (no data).

IT **753499-87-5P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of diazabicyclic aryl derivs. as cholinergic ligands at the nicotinic acetylcholine receptors)

RN 753499-87-5 ZCAPLUS
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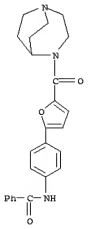

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L17 ANSWER 2 OF 2 ZCAPLUS COPYRIGHT 2009 ACS on STN
AN 2004:740327 ZCAPLUS
DN 141:260783
TI Preparation of diazabicyclic aryl derivatives as cholinergic ligands at the nicotinic acetylcholine receptors
IN Peters, Dan; Olsen, Gunnar M.; Nielsen, Elsebet Ostergaard; Jorgensen, Tino Dyhring; Ahring, Philip K.
PA Neurosearch A/S, Den.
SO PCT Int. Appl., 48 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

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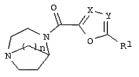

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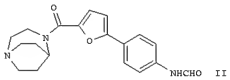

II

AB Title compds. represented by the formula I [wherein X, Y = independently CR2, CR3, N; R1 = H, (cyclo)alkyl, halo, etc.; R2, R3 = independently H, (cycloalkyl)alkyl, nitro, aryl, etc.; n = 1-3; and their enantiomers, any mixture of enantiomers, a prodrug, or pharmaceutically acceptable salts thereof] were prepared as cholinergic ligands at the nicotinic acetylcholine receptors. For example, reaction of (1,4-diazabicyclo[3.2.2]non-4-yl)-5-(4-aminophenyl)furan-2-ylmethanone and

=> d bib abs hitstr l18 tot

L18 ANSWER 1 OF 1 ZCAPLUS COPYRIGHT 2009 ACS on STN
AN 2004:740327 ZCAPLUS
DN 141:260783
TI Preparation of diazabicyclic aryl derivatives as cholinergic ligands at the nicotinic acetylcholine receptors
IN Peters, Dan; Olsen, Gunnar M.; Nielsen, Elsebet Ostergaard; Jorgensen, Tino Dyhring; Anring, Philip K.
PA Neurosearch A/S, Den.
SO PCT Int. Appl., 48 pp.
CODEN: PIXXD2
DT Patent
LA English
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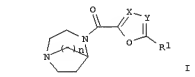

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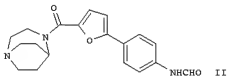
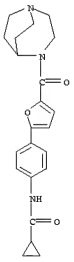


II

AB Title compds. represented by the formula I [wherein X, Y = independently CR2, CR3, N; R1 = H, (cyclo)alkyl, halo, etc.; R2, R3 = independently H, (cycloalkyl)alkyl, nitro, aryl, etc.; n = 1-3; and their enantiomers, any mixture of enantiomers, a prodrug, or pharmaceutically acceptable salts thereof] were prepared as cholinergic ligands at the nicotinic acetylcholine

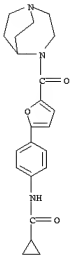
L18 ANSWER 1 OF 1 ZCAPLUS COPYRIGHT 2009 ACS on STN (Continued)



RN 753499-92-2 ZCAPLUS
CN Cyclopropanecarboxamide, N-[4-[5-(1,4-diazabicyclo[3.2.2]non-4-ylcarbonyl)-2-furanyl]phenyl]-, (2E)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

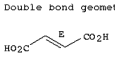
CRN 753499-91-1
CMF C22 H25 N3 O3



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

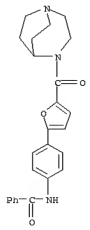


OSC.G 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)

L18 ANSWER 1 OF 1 ZCAPLUS COPYRIGHT 2009 ACS on STN (Continued)
receptors. For example, reaction of (1,4-diazabicyclo[3.2.2]non-4-yl)-5-(4-aminophenyl)furan-2-ylmethanone and Et formate gave II in 53% yield. II showed inhibition of 3H-α-Bungarotoxine binding with IC50 value of 0.017μM. Thus, I and their pharmaceutical compns. are useful as cholinergic ligands at the nicotinic acetylcholine receptors for the treatment of the central nervous system (CNS), the peripheral nervous system (PNS), diseases or disorders related to smooth muscle contraction, endocrine diseases or disorders, diseases or disorders related to neuro-degeneration, diseases or disorders related to inflammation, pain, and witndrawal symptoms caused by the termination of abuse of chem. substances (no data).
IT **753499-88-6P** **753499-91-1P** **753499-92-2P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of diazabicyclic aryl derivs. as cholinergic ligands at the nicotinic acetylcholine receptors)
RN 753499-88-6 ZCAPLUS
CN Benzamide, N-[4-[5-(1,4-diazabicyclo[3.2.2]non-4-ylcarbonyl)-2-furanyl]phenyl]-, (2E)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

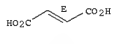
CRN 753499-87-5
CMF C25 H25 N3 O3



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



RN 753499-91-1 ZCAPLUS
CN Cyclopropanecarboxamide, N-[4-[5-(1,4-diazabicyclo[3.2.2]non-4-ylcarbonyl)-2-furanyl]phenyl]- (CA INDEX NAME)

L18 ANSWER 1 OF 1 ZCAPLUS COPYRIGHT 2009 ACS on STN (Continued)
RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L5              STR
L6          225 (NC5-NC2NC3 AND OC4)/ES
L7            2 L5 SAM SUB=L6
L8           14 L5 FULL SUB=L6
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L9           11 L8 AND L3
L10           3 L8 NOT L9
L11        2599 C25H25N3O3
L12           4 L11 AND L6
L13           3 L12 AND L3
L14           1 L12 NOT L13
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